# Theoretical Studies of Time Dependent/Independent Radiative Transfer Including Inelastic Scattering for Both Active and Passive Sources

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## LONG-TERM GOALS

We wish to develop the theoretical and computational groundwork for a new and innovative program for the remote detection and characterization of both organic and inorganic aerosols using both active (lidar) and passive techniques. This aerosol study should be very beneficial to the Navy in the areas of communications, high power laser transmission, air-sea interactions, and standoff biological detection methods. We also want to continue our collaborative program in polarimetry with the group in Minsk headed by Dr. Eleonora Zege.

#### **OBJECTIVES**

We will incorporate the full Mueller matrix formulation in this study to extract *everything* optically that can be extracted from the scattering and fluorescing aerosols. This study will also include the use of state-of-the-art techniques to calculate the single scattered Mueller matrix (SSMM) for both single particles as well as ensembles of particles that have different morphology and optical properties. We will show how to extend the SSMM into an "effective" multiple scattering Mueller matrix (MSMM) when multiple scattering has to be taken into account. We will also show that by using the MSMM it may be possible to not only determine particle optical properties and number densities but particle morphology as well. We will then determine which Mueller matrix elements or combination of them are most effective for unique aerosol signatures.

#### **APPROACH**

The success of this study for an active system depends on having programs to accurately calculate the complete time-resolved Mueller matrix for a realistic source-receiver geometry for a medium consisting of atmospheric gasses, clouds, and aerosols. We have already developed very powerful Monte Carlo programs that will calculate the multiple scattering Mueller matrix for any inhomogeneous atmosphere-ocean system which may contain a stochastic surface such as a dielectric interface separating the atmosphere from either a body of water or solid surface. These programs must be capable of handling not only backscattering (monostatic configuration), which is the most common mode of operation of lidar systems, but must also be able to handle any bistatic situation where source and receiver are at positions which will optimize the distinguishing feature of the aerosol under study.

We will first modify our existing state-of-the-art Monte Carlo codes to be able to handle both time dependent and time independent active sensing (see Kattawar and Rakovic, 1999; Rakovic and

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Form Approved OMB No. 0704-0188 Kattawar, 1998; and Rakovic, et al., 1999). For the lidar codes we will have the flexibility to have any source receiver geometry with arbitrary field of view (FOV) for the detector. This project is being worked on by Mr. Deric Gray who is doing his Ph.D. on this subject.

In addition to elastic scattering methods, it has been found that a very promising method for the detection of airborne biological aerosols (Biological Early Warning (BEW) designation) is through their fluorescence spectrum. This has been verified for earth-based spores such as *Bacillus subtilis* and *Bacillus anthracis* the causative agent for anthrax. We must add the fluorescent source to our Monte Carlo programs to handle this situation. In order to emulate fluorescence, we must do a broad wavelength coverage ranging from 350 nm - 680 nm. We have developed some nice techniques which will allow us to perform these multispectral calculations in a single computer run for certain situations. It is imperative that accurate calculations be made since the fluorescent signal, which will probably be weak, must always be compared to the ambient light also received by the detector. It should be noted that many organic aerosols may have virtually indistinguishable fluorescence spectra; however, this needs to be coupled to elastic scattering information to yield an unambiguous identification.

In order to run our Monte Carlo program, we still need the SSMM for the aerosols and other constituents comprising the atmospheric system. The actual experimental Mueller matrix data for aerosols of different shapes and optical properties are quite sparse at best, therefore we will have to develop our own computer codes to give us this data. Many aerosols whether from soils, minerals or organics can be highly nonspherical with large aspect ratios. Trying to model them with any type of equivalent sphere approximation can lead to substantial errors as has been pointed out by Mischenko et al., 1995,1997. There have been many techniques introduced to solve the problem of electromagnetic scattering from irregular particles (for an excellent summary of the methods the reader should see Mischenko, et al., 2000) the most notable of which are the discrete dipole approximation (DDA), the T-matrix approach, and the finite difference time domain method (FDTD). We have a good deal of experience with the DDA; however, even though it is capable of modeling any shape, it is quite limited to size parameters usually less than ten and also suffers from lack of accuracy in the Mueller matrix elements involving phase information. The T-matrix approach is very powerful and is able to achieve size parameters in excess of one hundred; however, it is not well suited for particles with sharp corners and edges where an inordinately large number of vector spherical wave functions may be needed. The FDTD method has a long and rich history beginning with the work of Yee, 1966. This method is applicable to any particle shape and inhomogeneity as well as handling any type of incident beam. The application of this method to effectively calculate light scattering properties from dielectric aerosols at a single frequency with a variety of shapes has been carried out by Yang, et al., 2000; however, virtually all comparisons were done on phase functions, the  $m_{11}$  element of the Mueller matrix, and is the least sensitive to numerical errors compared to all the other Mueller matrix elements. Since we will be interested in all the elements of the Mueller matrix, this may require modifying the type of boundary condition imposed (a crucial element in the accuracy of the FDTD) as well as a refinement of the discretization methods to yield the type of accuracy we need to produce the complete Mueller matrix. We want to extend the FDTD method to handle both dispersive and tensor permittivities as well. The reason being is that if one is using short pulsed sources the frequency spectrum can be quite wide and in most instances the permittivity will be a function of frequency and this behavior must be accounted for. Also most organic molecules and substances are optically active and therefore the permittivity will no longer be a scalar but will become a tensor. Both of these additions will involve extensive modification of the FDTD method as it presently exists.

It is therefore essential that we have a robust code to perform this type of calculation since Mueller matrix data for aerosols is very sparse and for bioaerosols virtually nonexistent. We will have to be able to effectively calculate the complete Mueller matrix for a single bacterium as well as spores, colonies, powders, etc. Another major difficulty is getting good optical properties for toxic bioaerosols in order to perform FDTD calculations. We will use data for simulants whenever possible. For example we will use optical properties for *Bacillus subtilis* to emulate *Bacillus anthracis*. We will thus be able to build a data bank of SSMM for both benign as well as lethal bioaerosols. Also for normal background aerosols we must be able to cover shapes from fluffy particles to spheres.

This project is being worked on by Pengwang Zhai and Changhui Li both of whom are Ph.D. students in the physics department of TAMU

## WORK COMPLETED

a) We have essentially completed a study of the effect of the shape of the volume scattering function on the detection of targets in turbid media. An extended abstract on this research has already been sent in for presentation at the Ocean Optics XVI conference in November

#### **RESULTS**

In Figures 1-4 we show the results of a Monte Carlo simulation of a circular target with three annular regions each with a different Mueller matrix for reflection embedded in a turbid medium similar to ocean water. The target was located at two optical depths from both the detector and source. We set the single scattering albedo of the medium to 0.50 and used five different phase functions to describe the scattering process. The rest of the Mueller matrix was taken to be similar to Rayleigh scattering. The five phase functions used have the following nomenclature on the graphs: A single term Henyey-Greenstein phase function with three different g values (SH), and a two-term Henyey-Greenstein with a large backscattering peak (TTHLBP) and a small backscattering peak (TTHSBP) respectively. The three dashed vertical lines in the figure show the boundaries of the annular regions with different Mueller matrices. Only the diagonal elements of the MSMM gave results different from zero. The explanation for this is quite complex and will not be addressed here.

# **Radiance** 0.009 0.008 0.007 Annular region boundaries 0.006 ← SH g=0.5 SH g = 0.80.005 SH g = 0.95TTH LBP 0.004 TTH SBP 0.003 0.002 0.001 $0.00\ 0.03\ 0.07\ 0.10\ 0.13\ 0.17\ 0.20\ 0.23\ 0.26\ 0.30\ 0.33\ 0.36\ 0.40$ **Distance from Target Center**

Fig. 1 Radiance as a function of distance from the target center for five different phase functions. As can be seen it would be very difficult if not impossible to "see" this low albedo target using just radiance data alone.

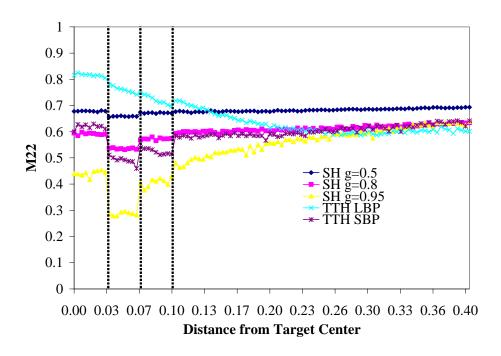


Fig. 2 Mueller matrix element M22 also as a function of distance from the target center. It should be noted that for most of the phase functions we can still "see" the surface features of the target.

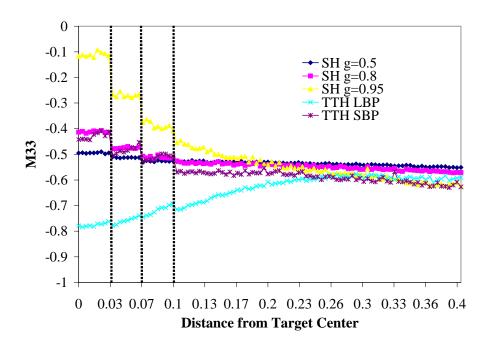


Fig. 3 Same as Fig. 2 except for the element M33. Note the separation in the continuum by g value and the fact that for the high g value (0.95) the effect of the target is seen all the way out to 0.26.

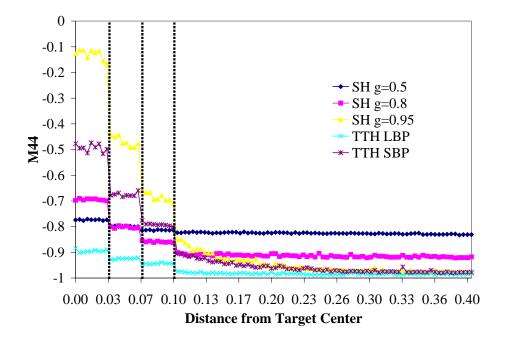


Fig. 4 Same as Fig. 2 except for the element M44. Note the large separation by different g values in the continuum and also the increased contrast in discerning surface features of the target\

#### IMPACT/APPLICATION

We now feel that from some of our preliminary work on Mueller matrix imaging, we will have new and more powerful tools for remotely sensing the atmosphere-ocean system. We also believe that it will lead to better and more comprehensive ways to detect and characterize both inorganic and bioaerosols such as anthrax spores.

Our Monte Carlo programs for laser scattering from turbid media are presently being used to study light scattering from living tissue. The only thing that is slowing the process is the fact that the Mueller matrix for both normal and malignant tissue is not known.

#### **TRANSITIONS**

Our Monte Carlo scalar code is being used to study the design of a new tube to measure both the scattering and absorption coefficients of seawater. This work is being done in collaboration with Dr. Ed Fry's group at TAMU and a patent application is now pending.

#### RELATED PROJECTS

Our inelastic scattering code is being used in a joint project with Dr. E. S. Fry to study the feasibility of using Brillouin scattering to measure the speed of sound as a function of depth in the ocean. This project is funded by the Texas Advanced Technology Program.

We are also using our passive Monte Carlo code to assist Dr. Walt McBride of PSI with a project to simulate complete pixel by pixel polarization imaging of targets in turbid media.

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# **PUBLICATIONS**

George W. Kattawar and Deric J. Gray, Influence of inherent optical properties on Mueller matrix imaging of targets in turbid media, to appear in Proceedings of OOXVI, 2003

Deric J. gray, George W. Kattawar, Edward S. Fry, Xianzchen Zhao, and Zheng Lu, An in situ device to directly measure both the absorption and scattering of the ocean waters, to appear in Proceedings of OOXVI, 2003

# **PATENTS**